

An Evaluation of Al Concentration Dependence of T_c in Two Gap Nature of $Mg_{1-x}Al_xB_2$ Superconductor

S. N. PANDEY* and L. K. MISHRA

*Village- Ankupur, P.O.- Belkhara Via-Usari Dist- Arawal-804428, Bihar, INDIA
Department of Physics,
Magadh University, Bodh-Gaya-824234, Bihar, INDIA

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ABSTRACT

In this paper, we have evaluated the Al concentration of T_c using electron phonon coupling constant and coulomb pseudo potential. Our theoretically evaluated results show that as doping concentration x (Al concentration) increases the zero field T_c decreases. This study shows that the σ bands collapsed gradually with Al doping due to the increase in the number of electrons. It was found that in all doping concentration the σ bands were dirtier than the π bands.

Keywords: two gap superconductor, clean limit, dirty limit, upper critical field, electron-phonon coupling parameter, Coulomb pseudo potential.

INTRODUCTION

The discovery of the relatively high T_c of 39 K in the very simple-structured magnesium diboride (MgB_2)¹ fascinated the scientific community. Soon after its discovery, MgB_2 was revealed to have a novel two-gap nature, which was found to influence its superconducting properties.²⁻⁶ Among these, the upper critical field (H_{c2}) was known to be affected seriously by the two-gap nature.⁷⁻¹¹ In the clean limit, at low temperatures H_{c2} and its anisotropy (γ_H) are

determined by the two- dimensional (2D) σ bands, while at high temperatures 3D π bands gradually became important in determining the H_{c2} and γ_H are mostly controlled by the amounts of the impurities,^{10,11} similar to the conventional one-gap BCS superconductors.^{12, 13} In MgB_2 however, there can be different scattering channels; within each band and between different pairs of bands. These are referred to as the intra band and inter band scatterings, respectively. According to the theory,^{10,11} inter band scattering allows the different gaps to merge,

simultaneously reducing the transition temperature. In the absence of the inter band scatterings, the H_{c2} and γ_H curves essentially depend on the intra band electron diffusivities. Near T_c , the H_{c2} curves are mainly determined by the diffusivities of the cleaner band between σ and π bands. On the other band, the zero-temperature $H_{c2}(0)$ is controlled by the dirtier band. This feature of two-gap superconductivity in the dirty limit causes the upward curvature near T_c and the significant enhancement of $H_{c2}(0)$ beyond the prediction of the one-gap BCS theory.^{10,14}

To address the above mentioned effects of the impurities, it should be noted that substituting Mg or B with other elements can differently affect the σ and π bands. It is expected that the B-site substitutions enhance the scattering within the σ bands, whereas Mg-site substitutions do the same thing in the π bands. of course, these can accompany the alterations of the electronic structure. However, detailed information on the modified electronic structure can be obtained in first principles calculation.^{15, 16} For instance, the main effect of Al doping in the Mg site was found to reduce the density of states at the Fermi level by increasing the number of electrons and to produced a band broadening by reducing the cell volume.¹⁵ However, even though several studies on Al-doped MgB_2 exist¹⁷⁻²⁰ the evolution of the impurity scattering with Al doping was not addressed until now.

In this work, we investigated the effect of Al doping on $H_{c2}(T)$ for $Mg_{1-x}Al_xB_2$ ($x=0, 0.1, 0.2, 0.3$). The $H_{c2}(T)$ values, determined by the resistivity measurements, were analysed by using the two-gap dirty-limit theory, along with the electron-phonon coupling constants and Coulomb pseudo potentials that were calculated in the first principles calculation.

The samples were synthesis in high-pressure and high temperature conditions. A stoichiometric mixture of Mg, B and Al powders was ground in a glove bag filled with inert Ar gas. The resulting precursor was pelletized, wrapped in Ta foil and put into a high pressure cubic cell. It was pressed up to 3.5 GPa and heat treated at 950°C for 2 h. It was then quenched to room temperature.

The structure of the samples was examined by x-ray diffraction measurements. The surface of morphology and the local compositions were investigated by using a field emission scanning electron microscope and energy dispersive spectroscopy, respectively.

2. MATHEMATICAL FORMULAE USED IN THE ANALYSIS

We used the theoretical formalism of A. Golubov and A.E. Koshelev^{10,11} of two-gap dirty limit theory of $H_{c2}(T)$ which takes the form in the absence of inter band scattering

$$a_o [\ln t + U(h)] [\ln t + U(\eta h)] + a_2 [\ln t + U(\eta h)] + a_1 [\ln t + U(\eta h) + U(h)] = 0 \quad (1)$$

Here

$$h = \frac{H_{c2} D_{\sigma}^{eff}}{2\Phi_0 T}$$

$$\eta = \frac{D_{\pi}^{eff}}{D_{\sigma}^{eff}}$$

$$U(x) = \psi\left(\frac{1}{2} + x\right) - \psi(x) \quad (2)$$

$\Psi(x)$ is the digamma function a_0, a_1, a_2 are the constants derived from the electron-phonon coupling constant (λ_{mn}^{ep}) and coulomb pseudo potential μ_{mn}

$$\lambda_{mn} = \lambda_{mn}^{ep} - \mu_{mn}$$

$$\Phi_0 = \text{flux quanta} \quad (3)$$

For the isotropic case, the electron diffusivity is given by $D = l v_F^2 / 3$ is the Fermi velocity and l is the electron mean free path. The numerical values of the data are given in table T₃.

If the system is sufficiently impure than the electronic mean free path l is much smaller than the coherence length ξ_0 of the pure material.

For dirty limit $\Delta \ll (1/\tau) \ll E_F$

For clean limit $l \gg \xi_0$ (4)

The electron diffusivities are actually related to the value of the resistivity. The resistivity can be expressed in terms of the electron diffusivities¹⁰ by

$$\frac{1}{\rho} = e^2 (N_{\sigma} D_{\sigma}^{eff} + N_{\pi} D_{\pi}^{eff}) \quad (5)$$

Where N_{π} and N_{σ} are the partial densities of states in the π and σ band respectively.

3. DISCUSSION OF RESULTS

In this paper, we have evaluated the Al concentration dependence of T_c in two gap nature of $Mg_{1-x}Al_xB_2$ superconductor. In table T₁ we have shown the Al concentration of T_c . The theoretical results were compared with the experimental data.¹⁵ Our theoretically evaluated results show that as x (Al-concentration) increases zero-field T_c decreases. This shows that σ bands collapse gradually with Al doping due to the increase in the number of electrons. At $x = 0.3$ an abrupt topological change of the σ bands in the open section of the Fermi surface was found. At $x = 0.6$ the σ bands vanishes completely. In table T₂, we have presented the temperature dependence of the H_{c2} at different doping concentration. From our theoretical results it appears that H_{c2} is highest at $x=0.0$ and lower for $x = 0.3$. For all doping $H_{c2}(T)$ decrease with T and at $T \rightarrow T_c$ its value tends to zero. In one gap BCS theory, $H_{c2}(T)$ enhances as the impurity scattering increase. In one gap BCS theory $H_{c2}(T)$ is linear near T_c . On the other hand in two gap nature of $Mg_{1-x}Al_xB_2$ superconductor as the Al contents increase both T_c and $H_{c2}(0)$ decrease. It shows that the three dimensional π bands become much dirtier when Al was doped. In contrast the inter band scattering of the two dimensional σ bands are relatively unaffected by the Al doping.^{25-30,}

The $H_{c2}(T)$ of $Mg_{1-x}Al_xB_2$ ($x = 0, 0.1, 0.2$ and 0.3) was studied based on the two-gap dirty-limit. The following facts were found:

1. The reduction of $H_{c2}(0)$ with x is related to the modifications of the electronic structure.
2. The 3D π band became much dirtier when the Al was doped, whereas the 2D σ bands were unaffected by such doping,
3. which indicates that Al doping is band sensitive when it acts as an impurity.
3. On examining over different doping concentrations, we have found that the σ bands were dirtier than the π bands.

Table T₁

An Evaluated results of Al concentration dependence of T_c for $Mg_{1-x}Al_xB_2$. The results were compared with experimental data¹⁵

Doping (x)	$T_c(K)$	
	Theory	Expt.
0.00	40.2	39.0
0.05	39.6	
0.10	38.4	36.5
0.15	34.2	
0.20	30.8	32.8
0.25	28.7	
0.30	26.5	28.4
0.35	24.8	
0.40	21.9	
0.45	19.8	
0.50	17.5	
0.55	11.2	
0.60	10.6	

Table T₂**An Evaluated results for temperature dependence of $H_{c2}(T)$ at different doping concentration**

T(K)	$H_{c2}(T)$			
	X = 0.0	X = 0.1	X = 0.2	X = 0.3
5	13.26	10.58	8.39	5.11
10	11.85	9.45	7.18	4.28
12	10.97	8.27	6.98	3.46
15	9.45	7.42	4.36	3.21
17	8.27	6.38	3.10	2.95
20	7.66	5.95	2.89	2.27
22	6.85	5.22	2.26	1.88
25	5.39	4.85	1.88	1.18
30	4.12	3.86	1.73	0.92
32	3.98	3.10	1.44	0.76
35	3.30	2.75	1.26	0.52
37	2.17	2.08	1.06	0.39
40	1.86	1.78	0.95	0.22

Table T₃**Parameter used in the calculation**

X	$\lambda_{\sigma\sigma}$	$\lambda_{\sigma\pi}$	$\lambda_{\pi\sigma}$	$\lambda_{\pi\pi}$	D_{π}^{eff} m^2S^{-1}	D_{σ}^{eff} m^2S^{-1}
0.0	0.810	0.119	0.090	0.285	7.0×10^{-3}	2.0×10^{-3}
0.1	0.670	0.170	0.115	0.366	6.0×10^{-3}	2.3×10^{-3}
0.2	0.511	0.185	0.121	0.395	1.7×10^{-3}	2.0×10^{-3}
0.3	0.407	0.166	0.145	0.376	1.1×10^{-3}	2.5×10^{-3}

X = doping concentration
 $\lambda_{\sigma\sigma}$ = coupling constant for $\sigma - \sigma$ band
 $\lambda_{\sigma\pi}$ = coupling constant for $\sigma - \pi$ band
 $\lambda_{\pi\sigma}$ = coupling constant for $\pi - \sigma$ band
 $\lambda_{\pi\pi}$ = coupling constant for $\pi - \pi$ band
 D_{π}^{eff} = Effective diffusivities for π band
 D_{σ}^{eff} = Effective diffusivities for σ band

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